



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:43 am BST

PDB ID : 6L93
Title : X-ray structure of the ligand-free human TRPV1 ankyrin repeat domain
Authors : Tanaka, M.; Hayakawa, K.; Unno, M.
Deposited on : 2019-11-08
Resolution : 4.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

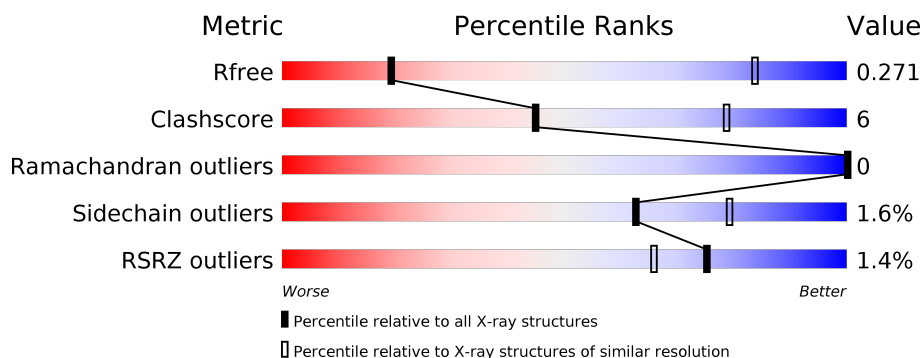
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1051 (5.12-3.80)
Clashscore	141614	1119 (5.12-3.80)
Ramachandran outliers	138981	1065 (5.12-3.80)
Sidechain outliers	138945	1047 (5.12-3.80)
RSRZ outliers	127900	1099 (5.20-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 71% 19% • 9% </div> </div>
1	B	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 70% 20% 9% </div> </div>
1	C	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 75% 16% 9% </div> </div>
1	D	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 79% 10% 10% </div> </div>
1	E	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 75% 15% 10% </div> </div>
1	F	280	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 3% <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 75% 15% 9% </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11813 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1974	1251	338	377	8			
1	B	254	Total	C	N	O	S	0	0	0
			1978	1253	339	378	8			
1	C	254	Total	C	N	O	S	0	0	0
			1978	1253	339	378	8			
1	D	251	Total	C	N	O	S	0	0	0
			1952	1237	333	374	8			
1	E	251	Total	C	N	O	S	0	0	0
			1953	1238	336	371	8			
1	F	254	Total	C	N	O	S	0	0	0
			1978	1253	339	378	8			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	expression tag	UNP Q8NER1
A	96	SER	-	expression tag	UNP Q8NER1
A	97	PRO	-	expression tag	UNP Q8NER1
A	98	ASN	-	expression tag	UNP Q8NER1
A	99	SER	-	expression tag	UNP Q8NER1
A	365	VAL	-	expression tag	UNP Q8NER1
A	366	ASP	-	expression tag	UNP Q8NER1
A	367	SER	-	expression tag	UNP Q8NER1
A	368	SER	-	expression tag	UNP Q8NER1
A	369	GLY	-	expression tag	UNP Q8NER1
A	370	ARG	-	expression tag	UNP Q8NER1
A	371	ILE	-	expression tag	UNP Q8NER1
A	372	VAL	-	expression tag	UNP Q8NER1
A	373	THR	-	expression tag	UNP Q8NER1
A	374	ASP	-	expression tag	UNP Q8NER1
B	95	GLY	-	expression tag	UNP Q8NER1

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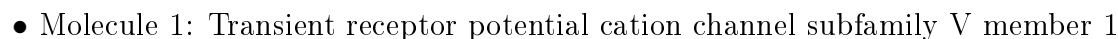
Chain	Residue	Modelled	Actual	Comment	Reference
B	96	SER	-	expression tag	UNP Q8NER1
B	97	PRO	-	expression tag	UNP Q8NER1
B	98	ASN	-	expression tag	UNP Q8NER1
B	99	SER	-	expression tag	UNP Q8NER1
B	365	VAL	-	expression tag	UNP Q8NER1
B	366	ASP	-	expression tag	UNP Q8NER1
B	367	SER	-	expression tag	UNP Q8NER1
B	368	SER	-	expression tag	UNP Q8NER1
B	369	GLY	-	expression tag	UNP Q8NER1
B	370	ARG	-	expression tag	UNP Q8NER1
B	371	ILE	-	expression tag	UNP Q8NER1
B	372	VAL	-	expression tag	UNP Q8NER1
B	373	THR	-	expression tag	UNP Q8NER1
B	374	ASP	-	expression tag	UNP Q8NER1
C	95	GLY	-	expression tag	UNP Q8NER1
C	96	SER	-	expression tag	UNP Q8NER1
C	97	PRO	-	expression tag	UNP Q8NER1
C	98	ASN	-	expression tag	UNP Q8NER1
C	99	SER	-	expression tag	UNP Q8NER1
C	365	VAL	-	expression tag	UNP Q8NER1
C	366	ASP	-	expression tag	UNP Q8NER1
C	367	SER	-	expression tag	UNP Q8NER1
C	368	SER	-	expression tag	UNP Q8NER1
C	369	GLY	-	expression tag	UNP Q8NER1
C	370	ARG	-	expression tag	UNP Q8NER1
C	371	ILE	-	expression tag	UNP Q8NER1
C	372	VAL	-	expression tag	UNP Q8NER1
C	373	THR	-	expression tag	UNP Q8NER1
C	374	ASP	-	expression tag	UNP Q8NER1
D	95	GLY	-	expression tag	UNP Q8NER1
D	96	SER	-	expression tag	UNP Q8NER1
D	97	PRO	-	expression tag	UNP Q8NER1
D	98	ASN	-	expression tag	UNP Q8NER1
D	99	SER	-	expression tag	UNP Q8NER1
D	365	VAL	-	expression tag	UNP Q8NER1
D	366	ASP	-	expression tag	UNP Q8NER1
D	367	SER	-	expression tag	UNP Q8NER1
D	368	SER	-	expression tag	UNP Q8NER1
D	369	GLY	-	expression tag	UNP Q8NER1
D	370	ARG	-	expression tag	UNP Q8NER1
D	371	ILE	-	expression tag	UNP Q8NER1
D	372	VAL	-	expression tag	UNP Q8NER1

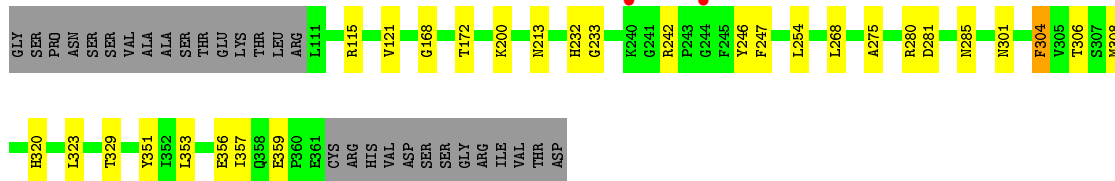
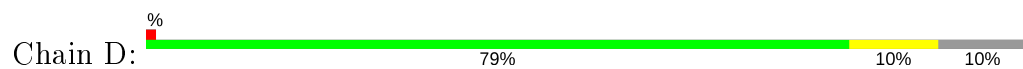
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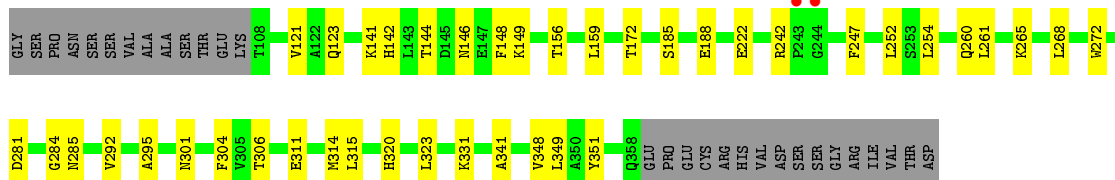
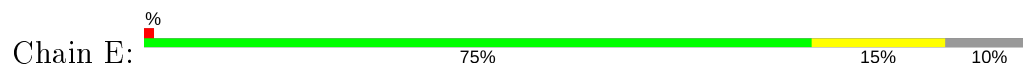
Chain	Residue	Modelled	Actual	Comment	Reference
D	373	THR	-	expression tag	UNP Q8NER1
D	374	ASP	-	expression tag	UNP Q8NER1
E	95	GLY	-	expression tag	UNP Q8NER1
E	96	SER	-	expression tag	UNP Q8NER1
E	97	PRO	-	expression tag	UNP Q8NER1
E	98	ASN	-	expression tag	UNP Q8NER1
E	99	SER	-	expression tag	UNP Q8NER1
E	365	VAL	-	expression tag	UNP Q8NER1
E	366	ASP	-	expression tag	UNP Q8NER1
E	367	SER	-	expression tag	UNP Q8NER1
E	368	SER	-	expression tag	UNP Q8NER1
E	369	GLY	-	expression tag	UNP Q8NER1
E	370	ARG	-	expression tag	UNP Q8NER1
E	371	ILE	-	expression tag	UNP Q8NER1
E	372	VAL	-	expression tag	UNP Q8NER1
E	373	THR	-	expression tag	UNP Q8NER1
E	374	ASP	-	expression tag	UNP Q8NER1
F	95	GLY	-	expression tag	UNP Q8NER1
F	96	SER	-	expression tag	UNP Q8NER1
F	97	PRO	-	expression tag	UNP Q8NER1
F	98	ASN	-	expression tag	UNP Q8NER1
F	99	SER	-	expression tag	UNP Q8NER1
F	365	VAL	-	expression tag	UNP Q8NER1
F	366	ASP	-	expression tag	UNP Q8NER1
F	367	SER	-	expression tag	UNP Q8NER1
F	368	SER	-	expression tag	UNP Q8NER1
F	369	GLY	-	expression tag	UNP Q8NER1
F	370	ARG	-	expression tag	UNP Q8NER1
F	371	ILE	-	expression tag	UNP Q8NER1
F	372	VAL	-	expression tag	UNP Q8NER1
F	373	THR	-	expression tag	UNP Q8NER1
F	374	ASP	-	expression tag	UNP Q8NER1

- Molecule 1: Transient receptor potential cation channel subfamily V member 1

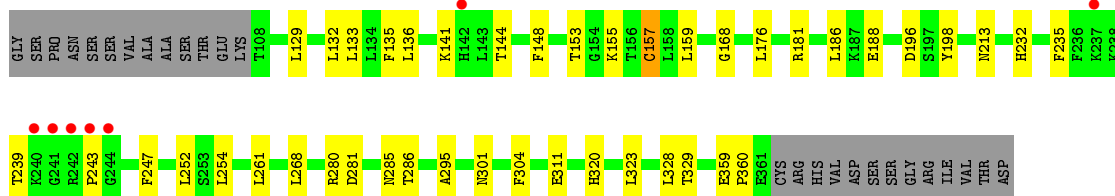
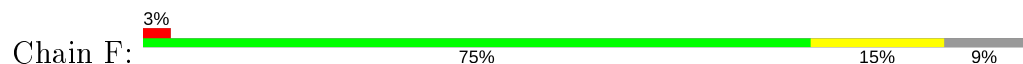




- Molecule 1: Transient receptor potential cation channel subfamily V member 1



- Molecule 1: Transient receptor potential cation channel subfamily V member 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.23Å 167.41Å 112.63Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	32.95 – 4.47 32.95 – 4.47	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.95-4.47) 90.4 (32.95-4.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 4.43Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.220 , 0.270 0.220 , 0.271	Depositor DCC
R_{free} test set	961 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	167.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11813	wwPDB-VP
Average B, all atoms (Å ²)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2004	0.43	0/2712
1	B	0.24	0/2008	0.42	0/2717
1	C	0.24	0/2008	0.41	0/2717
1	D	0.24	0/1982	0.41	0/2682
1	E	0.24	0/1982	0.42	0/2681
1	F	0.24	0/2008	0.43	0/2717
All	All	0.24	0/11992	0.42	0/16226

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1974	0	2008	41	0
1	B	1978	0	2014	34	0
1	C	1978	0	2014	25	0
1	D	1952	0	1983	16	0
1	E	1953	0	1995	23	0
1	F	1978	0	2014	21	0
All	All	11813	0	12028	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD13	1:A:355:ARG:NH1	1.93	0.82
1:A:313:LEU:HD13	1:A:355:ARG:CZ	2.14	0.77
1:A:313:LEU:CD1	1:A:355:ARG:NH2	2.55	0.69
1:A:133:LEU:HD13	1:A:179:ILE:HD12	1.75	0.69
1:A:173:ILE:HG13	1:A:174:PRO:HD3	1.76	0.67
1:B:219:LEU:O	1:B:223:ASN:ND2	2.27	0.66
1:A:117:ILE:HG12	1:A:132:LEU:HD22	1.78	0.66
1:A:143:LEU:HB3	1:A:189:LEU:HD11	1.77	0.66
1:A:162:MET:HB3	1:A:207:ILE:HG21	1.77	0.66
1:B:153:THR:HA	1:B:196:ASP:HB3	1.76	0.66
1:A:313:LEU:HD13	1:A:355:ARG:NH2	2.11	0.65
1:B:126:CYS:HG	1:B:171:THR:HG1	1.43	0.65
1:A:313:LEU:O	1:A:313:LEU:HD23	1.97	0.64
1:A:261:LEU:HD11	1:A:311:GLU:HG2	1.78	0.64
1:C:219:LEU:O	1:C:223:ASN:ND2	2.31	0.63
1:E:247:PHE:HB2	1:E:254:LEU:HA	1.79	0.63
1:A:313:LEU:HD13	1:A:355:ARG:HH12	1.63	0.61
1:E:121:VAL:HG13	1:E:172:THR:HG21	1.82	0.61
1:E:142:HIS:CE1	1:E:185:SER:HB3	2.35	0.61
1:F:168:GLY:O	1:F:213:ASN:ND2	2.33	0.61
1:F:280:ARG:NH1	1:F:329:THR:O	2.28	0.61
1:A:260:GLN:HB3	1:A:263:ILE:HD13	1.83	0.60
1:D:280:ARG:NH1	1:D:329:THR:O	2.33	0.59
1:D:242:ARG:NH2	1:E:123:GLN:O	2.35	0.59
1:E:320:HIS:HB3	1:E:323:LEU:HD23	1.84	0.59
1:C:247:PHE:HB2	1:C:254:LEU:HA	1.85	0.59
1:A:313:LEU:HD11	1:A:355:ARG:NH2	2.19	0.57
1:B:168:GLY:O	1:B:213:ASN:ND2	2.32	0.57
1:F:295:ALA:HA	1:F:301:ASN:HD21	1.68	0.57
1:A:288:LEU:HD12	1:A:336:PRO:HB3	1.87	0.56
1:D:281:ASP:OD1	1:D:285:ASN:N	2.39	0.56
1:A:173:ILE:HG13	1:A:174:PRO:CD	2.35	0.56
1:B:280:ARG:NH1	1:B:329:THR:O	2.32	0.56
1:B:281:ASP:OD1	1:B:285:ASN:N	2.38	0.55
1:D:168:GLY:O	1:D:213:ASN:ND2	2.35	0.55
1:A:219:LEU:O	1:A:223:ASN:ND2	2.33	0.55
1:A:296:ASP:H	1:A:301:ASN:ND2	2.04	0.54
1:E:295:ALA:HA	1:E:301:ASN:HD21	1.72	0.54
1:A:296:ASP:H	1:A:301:ASN:HD21	1.55	0.54
1:A:170:ASN:HB3	1:A:173:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ARG:NH2	1:C:329:THR:O	2.40	0.54
1:F:320:HIS:HB3	1:F:323:LEU:HD23	1.90	0.54
1:A:175:LEU:O	1:A:179:ILE:HG12	2.08	0.54
1:F:155:LYS:HA	1:F:159:LEU:HD12	1.90	0.54
1:F:286:THR:HG21	1:F:328:LEU:HD11	1.89	0.54
1:A:313:LEU:CD1	1:A:355:ARG:HH22	2.20	0.54
1:D:121:VAL:HG13	1:D:172:THR:HG21	1.91	0.53
1:A:155:LYS:HD3	1:A:160:LYS:HD3	1.91	0.53
1:D:246:TYR:OH	1:D:281:ASP:OD2	2.24	0.53
1:D:247:PHE:HB2	1:D:254:LEU:HA	1.90	0.53
1:A:238:LYS:NZ	1:A:239:THR:O	2.40	0.52
1:F:133:LEU:O	1:F:136:LEU:HD23	2.09	0.52
1:E:281:ASP:OD1	1:E:285:ASN:N	2.42	0.52
1:A:252:LEU:HD11	1:A:268:LEU:HD21	1.92	0.51
1:D:320:HIS:HB3	1:D:323:LEU:HD23	1.91	0.51
1:B:133:LEU:HD13	1:B:179:ILE:HG23	1.92	0.51
1:A:179:ILE:O	1:A:183:THR:OG1	2.24	0.51
1:A:205:LEU:O	1:A:209:ILE:HG12	2.11	0.51
1:C:149:LYS:HG2	1:C:156:THR:HG22	1.92	0.51
1:F:252:LEU:HD11	1:F:268:LEU:HD21	1.92	0.51
1:C:252:LEU:HD11	1:C:268:LEU:HD21	1.92	0.51
1:B:292:VAL:HG22	1:B:348:VAL:HG11	1.93	0.50
1:B:350:ALA:HB2	1:C:349:LEU:HD11	1.94	0.50
1:A:281:ASP:OD1	1:A:285:ASN:N	2.45	0.50
1:D:356:GLU:HA	1:D:359:GLU:HG3	1.94	0.49
1:B:155:LYS:HA	1:B:159:LEU:HD12	1.95	0.49
1:B:252:LEU:HD11	1:B:268:LEU:HD21	1.93	0.49
1:E:252:LEU:HD11	1:E:268:LEU:HD21	1.95	0.49
1:B:165:LEU:HD12	1:B:211:ARG:HH21	1.78	0.48
1:C:113:ASP:OD1	1:C:113:ASP:N	2.46	0.48
1:C:350:ALA:HB2	1:E:349:LEU:HD11	1.94	0.48
1:C:239:THR:HG21	1:C:244:GLY:H	1.79	0.48
1:C:281:ASP:OD1	1:C:285:ASN:N	2.46	0.48
1:E:156:THR:H	1:E:159:LEU:HD12	1.79	0.48
1:F:261:LEU:HD21	1:F:311:GLU:HG2	1.96	0.47
1:B:295:ALA:HA	1:B:301:ASN:HD21	1.79	0.47
1:E:142:HIS:HE1	1:E:185:SER:HB3	1.78	0.47
1:F:129:LEU:HD22	1:F:132:LEU:HD22	1.96	0.47
1:A:222:GLU:HG2	1:A:272:TRP:NE1	2.30	0.47
1:D:301:ASN:HA	1:D:304:PHE:HD2	1.79	0.47
1:B:144:THR:HG21	1:B:188:GLU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:GLY:HA3	1:E:331:LYS:HB2	1.97	0.47
1:F:144:THR:HG21	1:F:188:GLU:HB3	1.97	0.46
1:E:265:LYS:HG2	1:E:315:LEU:HD21	1.95	0.46
1:B:247:PHE:HB2	1:B:254:LEU:HA	1.97	0.46
1:F:132:LEU:O	1:F:135:PHE:HB3	2.15	0.46
1:A:155:LYS:HA	1:A:159:LEU:HD12	1.96	0.46
1:C:237:LYS:HG2	1:C:238:LYS:H	1.80	0.46
1:A:239:THR:HG22	1:A:243:PRO:HA	1.98	0.46
1:B:121:VAL:HG13	1:B:172:THR:HG21	1.96	0.46
1:F:247:PHE:HB2	1:F:254:LEU:HA	1.98	0.46
1:B:126:CYS:SG	1:B:171:THR:OG1	2.60	0.45
1:C:292:VAL:O	1:C:345:LYS:NZ	2.46	0.45
1:A:132:LEU:HA	1:A:135:PHE:HB3	1.99	0.45
1:A:246:TYR:OH	1:A:281:ASP:OD2	2.30	0.45
1:B:242:ARG:HA	1:B:242:ARG:HD3	1.80	0.45
1:E:141:LYS:HD3	1:E:148:PHE:HZ	1.81	0.45
1:D:115:ARG:HA	1:D:115:ARG:HH11	1.81	0.45
1:C:310:ASN:HB2	1:C:351:TYR:OH	2.17	0.45
1:F:141:LYS:HD3	1:F:148:PHE:HZ	1.80	0.45
1:B:144:THR:HG23	1:B:185:SER:HB3	1.99	0.45
1:E:222:GLU:HG2	1:E:272:TRP:CE2	2.51	0.45
1:A:114:ARG:NH1	1:A:149:LYS:O	2.51	0.44
1:F:359:GLU:OE1	1:F:360:PRO:HD3	2.17	0.44
1:C:186:LEU:HD11	1:C:223:ASN:HB3	1.98	0.44
1:A:239:THR:OG1	1:A:240:LYS:N	2.51	0.44
1:C:239:THR:HG21	1:C:243:PRO:HA	1.99	0.44
1:C:261:LEU:HD21	1:C:311:GLU:HG2	1.99	0.44
1:E:292:VAL:HG22	1:E:348:VAL:HG11	1.99	0.44
1:B:193:SER:HB3	1:B:203:THR:HG22	1.98	0.44
1:F:153:THR:HA	1:F:196:ASP:HB3	2.00	0.44
1:B:121:VAL:HG22	1:B:172:THR:HG21	2.00	0.44
1:F:239:THR:HG21	1:F:243:PRO:HA	2.00	0.43
1:A:288:LEU:HD22	1:A:288:LEU:HA	1.80	0.43
1:C:198:TYR:OH	1:C:242:ARG:NH1	2.51	0.43
1:B:292:VAL:O	1:B:345:LYS:NZ	2.47	0.43
1:D:268:LEU:HD23	1:D:275:ALA:HB3	2.01	0.43
1:A:288:LEU:HD11	1:A:309:TYR:CE2	2.54	0.43
1:B:187:LYS:HA	1:B:190:VAL:HG12	2.01	0.43
1:E:261:LEU:HD21	1:E:311:GLU:HG2	2.01	0.43
1:B:200:LYS:HB3	1:B:233:GLY:HA2	2.00	0.43
1:B:320:HIS:HB3	1:B:323:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LYS:HA	1:C:159:LEU:HD12	2.01	0.43
1:A:115:ARG:HG2	1:B:211:ARG:HD3	2.01	0.43
1:C:306:THR:HG23	1:C:351:TYR:CE2	2.54	0.43
1:E:144:THR:HG21	1:E:188:GLU:HB2	2.01	0.42
1:C:285:ASN:HB3	1:C:289:HIS:HB2	2.00	0.42
1:D:301:ASN:HA	1:D:304:PHE:CD2	2.54	0.42
1:B:306:THR:HG23	1:B:351:TYR:CE2	2.54	0.42
1:B:354:GLN:O	1:B:358:GLN:HG2	2.19	0.42
1:D:353:LEU:O	1:D:357:ILE:HG13	2.19	0.42
1:B:120:ALA:HA	1:B:123:GLN:HE21	1.83	0.42
1:B:239:THR:OG1	1:B:240:LYS:N	2.52	0.42
1:E:149:LYS:HG2	1:E:156:THR:HG22	2.01	0.42
1:C:288:LEU:HD11	1:C:325:LEU:HB3	2.02	0.42
1:D:306:THR:HG23	1:D:351:TYR:CD2	2.54	0.42
1:B:301:ASN:HA	1:B:304:PHE:CD1	2.55	0.42
1:A:265:LYS:HG2	1:A:315:LEU:HD21	2.02	0.42
1:E:311:GLU:HA	1:E:314:MET:HG2	2.02	0.42
1:F:157:CYS:SG	1:F:176:LEU:HD21	2.60	0.42
1:F:181:ARG:HA	1:F:186:LEU:HB2	2.01	0.42
1:A:144:THR:HG21	1:A:188:GLU:HB2	2.02	0.41
1:B:246:TYR:OH	1:B:281:ASP:OD2	2.25	0.41
1:B:222:GLU:HG2	1:B:272:TRP:NE1	2.35	0.41
1:C:121:VAL:HG22	1:C:172:THR:HG21	2.02	0.41
1:E:146:ASN:HA	1:E:149:LYS:HE2	2.01	0.41
1:A:277:ILE:HD11	1:A:312:ILE:HG23	2.01	0.41
1:B:301:ASN:HA	1:B:304:PHE:HD1	1.86	0.41
1:D:200:LYS:HB3	1:D:233:GLY:HA2	2.02	0.41
1:C:347:GLY:HA2	1:E:341:ALA:HB1	2.03	0.40
1:C:298:THR:OG1	1:C:301:ASN:HB3	2.22	0.40
1:C:112:TYR:HE2	1:C:131:SER:HB3	1.87	0.40
1:E:306:THR:HG23	1:E:351:TYR:CE2	2.57	0.40
1:F:198:TYR:CE2	1:F:235:PHE:HB2	2.56	0.40
1:F:281:ASP:OD1	1:F:285:ASN:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/280 (90%)	244 (97%)	8 (3%)	0	100	100
1	B	252/280 (90%)	245 (97%)	7 (3%)	0	100	100
1	C	252/280 (90%)	246 (98%)	6 (2%)	0	100	100
1	D	249/280 (89%)	238 (96%)	11 (4%)	0	100	100
1	E	249/280 (89%)	239 (96%)	10 (4%)	0	100	100
1	F	252/280 (90%)	243 (96%)	9 (4%)	0	100	100
All	All	1506/1680 (90%)	1455 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/237 (90%)	209 (98%)	5 (2%)	50	70
1	B	215/237 (91%)	211 (98%)	4 (2%)	57	75
1	C	215/237 (91%)	213 (99%)	2 (1%)	78	87
1	D	212/237 (90%)	209 (99%)	3 (1%)	67	81
1	E	212/237 (90%)	209 (99%)	3 (1%)	67	81
1	F	215/237 (91%)	212 (99%)	3 (1%)	67	81
All	All	1283/1422 (90%)	1263 (98%)	20 (2%)	62	79

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	236	PHE
1	A	301	ASN
1	A	308	MET
1	A	309	TYR
1	B	214	MET
1	B	232	HIS
1	B	304	PHE
1	B	308	MET
1	C	234	ASP
1	C	304	PHE
1	D	232	HIS
1	D	304	PHE
1	D	308	MET
1	E	242	ARG
1	E	260	GLN
1	E	304	PHE
1	F	157	CYS
1	F	232	HIS
1	F	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	GLN
1	E	142	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	254/280 (90%)	-0.33	2 (0%)	86 79	125, 165, 222, 267	0
1	B	254/280 (90%)	-0.35	4 (1%)	72 63	124, 164, 208, 279	0
1	C	254/280 (90%)	-0.31	4 (1%)	72 63	123, 177, 224, 282	0
1	D	251/280 (89%)	-0.23	2 (0%)	86 79	139, 188, 242, 272	0
1	E	251/280 (89%)	-0.34	2 (0%)	86 79	131, 184, 231, 282	0
1	F	254/280 (90%)	-0.10	7 (2%)	53 43	129, 205, 257, 272	0
All	All	1518/1680 (90%)	-0.28	21 (1%)	75 66	123, 179, 243, 282	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	243	PRO	4.9
1	F	244	GLY	4.3
1	E	244	GLY	3.8
1	B	243	PRO	3.6
1	F	242	ARG	3.6
1	B	244	GLY	3.6
1	C	243	PRO	3.5
1	E	243	PRO	3.3
1	D	240	LYS	3.3
1	D	244	GLY	3.3
1	F	241	GLY	3.3
1	C	240	LYS	2.5
1	F	240	LYS	2.5
1	B	240	LYS	2.4
1	A	234	ASP	2.3
1	F	237	LYS	2.3
1	C	241	GLY	2.2
1	C	110	ARG	2.1
1	F	142	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	ARG	2.1
1	B	241	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.